GE(LI) DATA REDUCTION USING SMALL COMPUTERS

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1. INTRODUCTION

The introduction of lithium-drifted germanium detectors for use in X-ray and gamma ray spectroscopy has made it possible to measure accurately the relative abundances of radionuclides present in a mixture directly, without the use of chemical separation techniques. Events depositing differing amounts of emergy into the crystal result in pulses of varied height,which are then sorted using a pulse height analyzer. Having accumulated a spectrum, three steps are required for its analysis. The peaks in the spectrum must be found, the count rate in the photopeaks determined, and this count rate related through a knowledge of machine efficiencies to known gamma transitions to find the amount of each radionuclide present. Since 4096 channels of data are usually involved, this process has often been accomplished on a remote computer. With the introduction of small , relatively inexpensive computers it has become possible to interface these devices with the Ge(Li) detector in such a way as to allow the experimenter to maintain an interactive control not only of the experimental parameters, but also of the data interpretation. This latter approach also has the desirable advantage of providing real-time information on the progress of the experiment.

There are essentially two approaches which are used to produce an interactive system. In the first, the small computer is interfaced directly to the ADC and a portion of the computer memory provides the storage area for the data; whereas in the second, the computer is interfaced to the analyzer memory in which the data is stored. The analyzer memory thus appears to the central processor as a bulk storage device. We have pursued the latter approach.

2. ANALYZER/COMPUTER COMBINATION

The system used in this study was a commerically made <u>50/50 System</u> , obtained from NUCLEAR DATA. It includes a 100 MHz ADC with 8192 resolution and a 4096 word, 24 bit analyzer memory. Also part of this system was a 12K PDP 8/I computer produced by DIGITAL EQUIPMENT CORP. Other equipment included a display scope, high speed punch/reader unit, teletype, and interface units. Machine language instructions were provided to control all major functions of the analyzer under computer control,as well as allowing acess through the computer accumulator to any memory location within the analyzer or direct access to the ADC output.

Various computing languages are available to program the PDP 8/I;including assembly languages, FORTRAN, and FOCAL (a conversational language). The assembly languages are most efficient from the point of view of speed and program size,however,programs are long and tedious to write. FOCAL requires the compiler to reside in core and is therefore wasteful of core memory. FORTRAN programs allow easier design and modification and also eliminate training operators in the assembly languages. Furthermore, FORTRAN programs are available from a variety of sources including the excellent text by Bevington (ref. 1). Our approach was to utilize FORTRAN programs with a number of FORTRAN-callable routines which provide control over the major functions of the analyzer.

3. LIMITATIONS OF FORTRAN

There are several limitations placed on the FORTRAN program by the construction of the central processor. The PDP 8/I memory is divided into 4096 word units called <u>fields</u> . Each field is further divided into 128 word blocks called <u>pages</u>. There are 32 pages in a field. The FORTRAN loader requires 3 pages in the first field (field 0), and one page each in the remaining fields. Some locations in the first page in each field are also required leaving 27 pages available in field 0 and 30 in each of the remaining fields. The FORTRAN library subroutines; including subscripting,square root,read,write,add, subtract, etc. requires another 25 pages. The exponentiation routines are not included and would require another 6 pages. Without the latter, in a 12K computer, this leaves 62 free pages or about 8K for operator programs.

4. SERVICE ROUTINES

Four service routines were written to facilitate analysis of the Ge(Li) spectrum. These are listed on Slide 1. The routines ANAL and TYME are in the same package and occupy 2 pages of core, as does each of the other routines.

5. METHODS OF ANALYSIS

The general problem in the analysis

of Ge(Li) spectra is to determine the area of the full energy photopeak after subtraction of the background, which is due to Compton interactions produced by higher energy gammas. The main portion of the photopeak is a gaussian function, modified on the low energy side by tailing. A close examination of well defined photopeaks, such as the one shown on Slide 2, also reveals the existence of a step function-like contribution, the higher level of which is again on the low energy side of the photopeak. The actual situation is not as bad as shown as the scale is semi-logarithmic.

In the case of isolated photopeaks, the photopeak area is simply what is left over after the background is subtracted so the problem reduces to a determination of the form of the background. One possible approach is to define a region on either side of the peak and draw a least square straight line through it. The photopeak is defined as anything above that line. A more pleasing solution might be to join the two regions on either side of the peak by a smooth function such as $(1 - \mathrm{erf}(x))$. With a small computer, however, it is more practical to use the former method. The error resulting from using this method is about 1%.

When photopeaks are not isolated, then there is a second problem - that of determining how much of the total peak area is due to a specific gamma ray. For this it is necessary to use an expression for the individual peak shapes and an iterative procedure to minimize the weighted squared error (chisquare). The error in this type of determination is proportional to the product of chisquare and the error expected from Poisson statistics alone. Either of these types of analysis can be coded in FORTRAN and run on the 50/50 system described earlier.

6. ANALYSIS PROGRAM

A flow chart of a typical peak location and analysis program is shown on the next slide. An initial set of parameters is read in from the high speed paper tape reader. These include smoothing coefficients for the peak finding routine, gain, zero, and estimates of the peak width as a function of channel number. The teletype is then used to define the region to be analyzed, the minimum separation between isolated peaks, and the number of channels to be used in the background region. The photopeaks are then found by the subroutine FIND which examines the behavior of the smoothed first derivative of the spectrum using an algorithmn similar to that used in the GASPAN program (ref 2). When all peaks have been found, the first (highest energy) peak is checked against the second to determine if they are resolved. If so, the specified number of channels are extracted from the analyzer and the limits of the peak determined. The program looks on either side of the peak for three successive increases in the smoothed channel contents such that the difference between the first and third values are at least twice the square root of the first. The first channel in this group is taken to be the limit of the peak on that side. The remaining channels are then used to calculate a least square line to be used as the background and the resulting peak area and centroid calculated.

If the peak was found not to be isolated, then the region to be analyzed includes that second peak and any other unresolved peaks. After calculating the total peak area in the same manner as for an isolated peak, a non-linear least square fit using the functional form:

$$y = a + bx + \sum_{1}^{4} c_i \exp(- s^2 (x-d_i)^2)$$

is used and the total area for each peak calculated from the area previously calculated and the relative peak amplitude. The form of the functional fit may be varied by using different calculation subprograms. The next slide shows a memory map of this program to give some idea of the size of each subprogram.

7. CONCLUSION

In conclusion, I feel that a small computer can perform the first two steps necessary in the analysis of a Ge(Li) spectrum. The last step, that of correlating the photopeak intensities and determining the amount of each radionuclide present must be taken either by the experimenter or a larger computer.

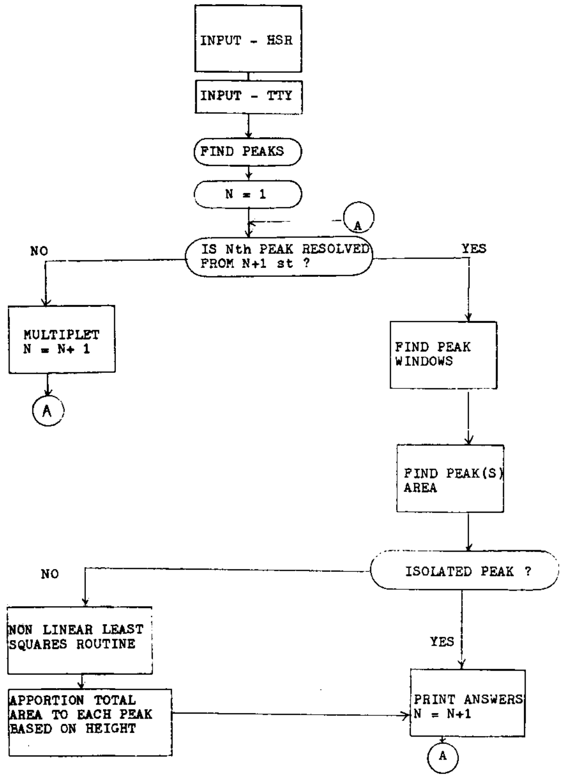
REFERENCES

1. Bevington, P.R. : Data Reduction and Error Analysis for the Physical Sciences. McGraw-Hill (1969)

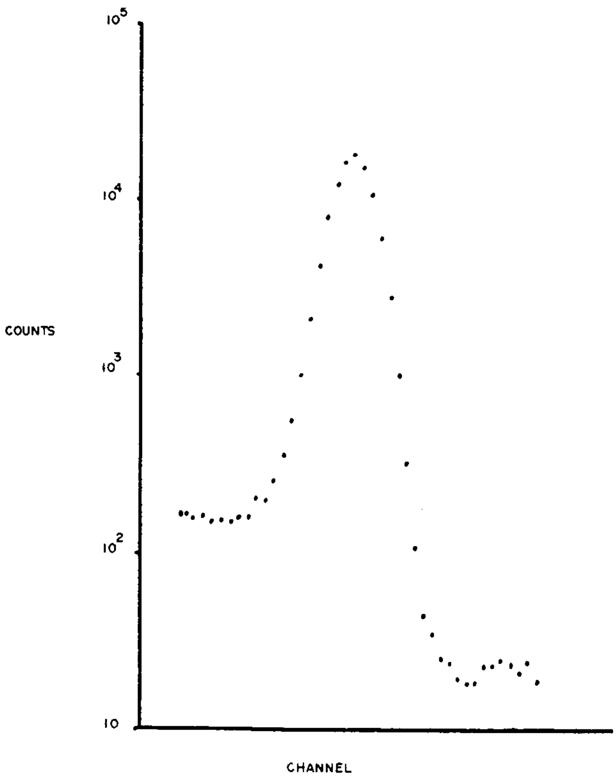
2. Barnes, V.: IEEE Trans.Nucl.Sci. NS-15, no 3 (1968)

SLIDE 1 FORTRAN SERVICE ROUTINES

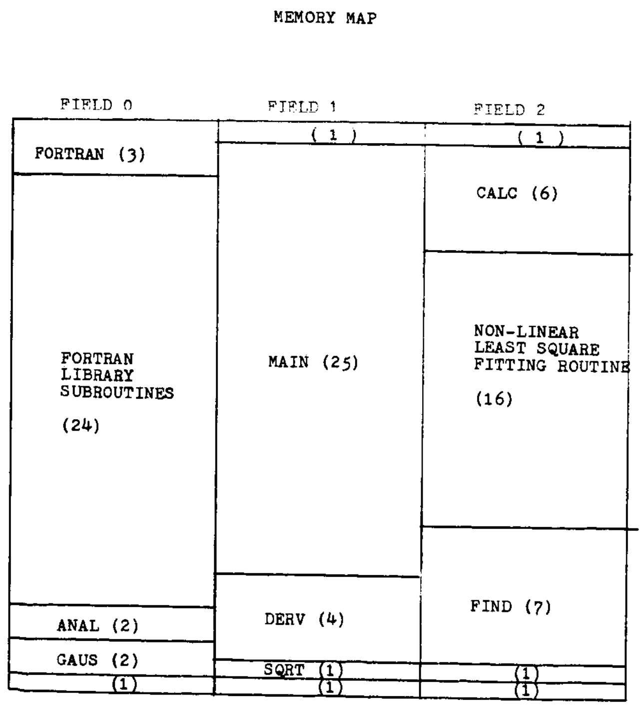
Name	Calling Statement	
ANAL	CALL ANAL (CTS,CHAN,N)	Load into the vector CTS, starting at CTS(1), the contents of the N analyzer locations beginning with CHAN. Convert 24 bit word to floating point.
TYME	X=TYME(T)	Load contents of analyzer channel 0 into X after converting to floating point and multiplying by the constant T.
FNDIL	CALL FNDIL (X,Y)	Find the upper channel, X, and the lower channel, Y, of the analog intensified region on the display scope.
GAUS	X = GAUS (T)	Compute EXP($-T^2$). If T is greater in magnitude than 5, GAUS (T) = 0.



SLIDE 3



SLIDE 2



SLIDE 4